PERTURBO: A software platform for accelerated discovery of microscopic processes in materials

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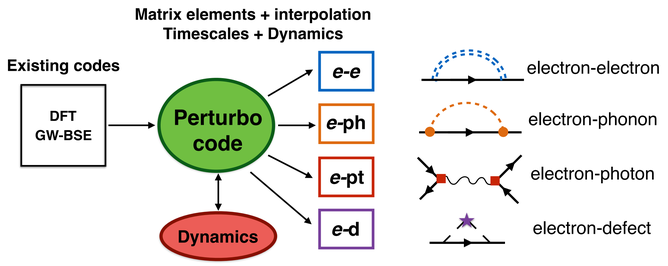
Introduction

- Solid-state technologies depend crucially on **charge carrier scattering and dynamics.** Charge carriers are scattered by quasiparticles and excitations in materials (e.g. phonons, defects, photons, electrons, holes, etc.)
- PERTURBO is a robust platform to study these electron scattering processes using **first-principles calculations and many-body perturbation theory**. PERTURBO fills a void in the software ecosystem to design advanced materials, and will foster scientific and technological innovation.



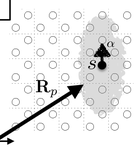
- PERTURBO combines **new computational methods** developed in our group. The code implementation adopts **modern programming practices** (HDF5, version control, MPI/OpenMP) and will be distributed under the standard open GPL license.

Example: electron-phonon scattering

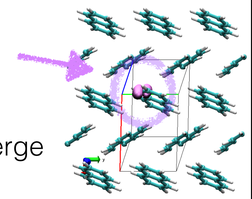
- The electron-phonon (e-ph) coupling matrix element ***g***:

$$g^{\mathbf{q}s\alpha,mn}_{\mathbf{k}+\mathbf{q},\mathbf{k}} = \langle \psi_{m\mathbf{k}+\mathbf{q}} | \partial^{s\alpha}_{\mathbf{q}} V(\mathbf{r}) | \psi_{n\mathbf{k}} \rangle$$

$$\partial^{s\alpha}_{\mathbf{q}} V(\mathbf{r}) = \sum_{\mathbf{R}_p} e^{i\mathbf{q}\cdot\mathbf{R}_p} \partial_{\mathbf{R}_p,s\alpha} V(\mathbf{r})$$



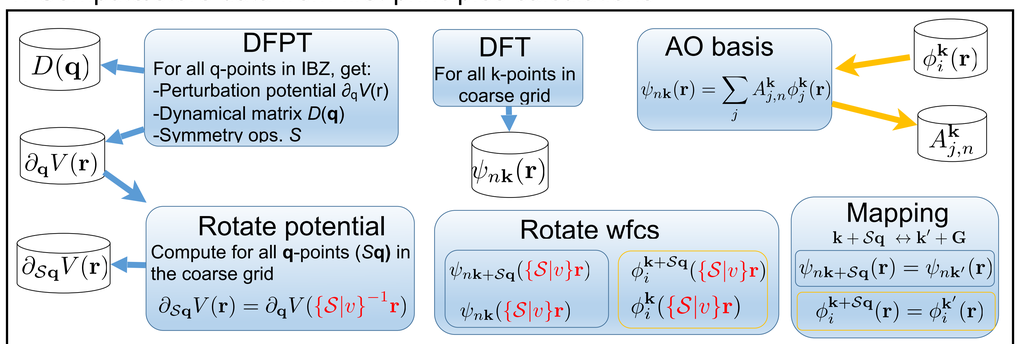
- DFT: electron wavefuncs. $\psi_{m\mathbf{k}+\mathbf{q}}, \psi_{n\mathbf{k}}$ from first principles
- DFPT: Perturbation $\partial^{s\alpha}_{\mathbf{q}} V(\mathbf{r})$ due to a phonon with wavevector **q**
- Need > **10^6** **q** and **k** points to converge charge carrier transport properties



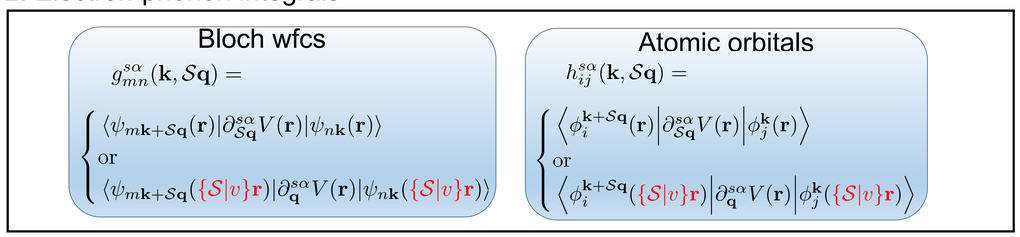
- An interpolation scheme is needed to evaluate ***g(k,q)*** on ultrafine **k** and **q** grids

Interpolation of the e-ph coupling with atomic orbitals (AOs)

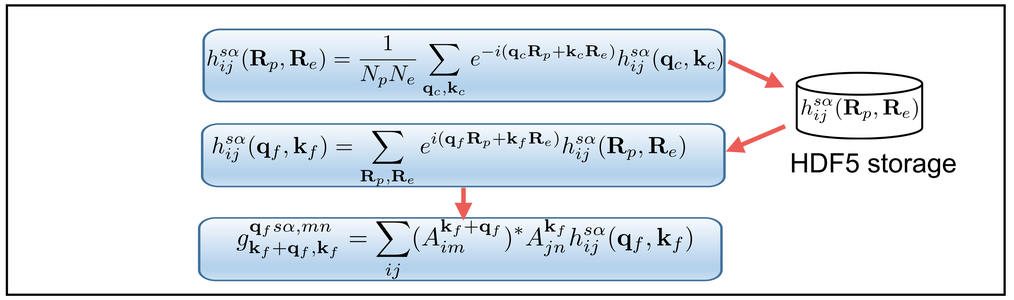
1. Compute/store data from first-principles calculations



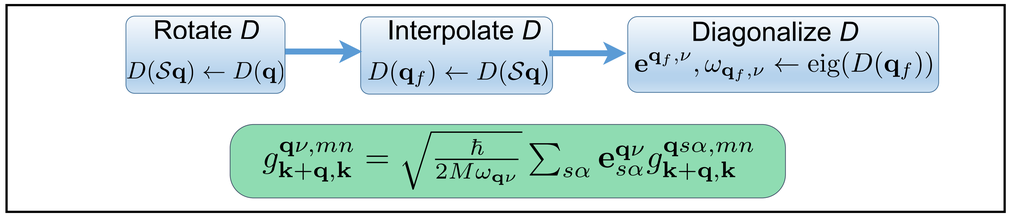
2. Electron-phonon integrals



3. Interpolation to fine grids ($\mathbf{k}_f$, $\mathbf{q}_f$) with atomic orbitals



3. Electron-phonon coupling on the fine grid ($\mathbf{k}_f$, $\mathbf{q}_f$)

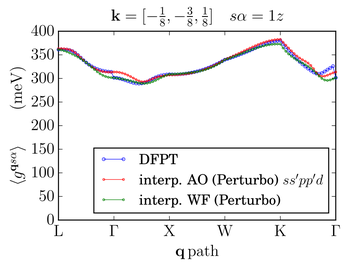


4. Compute the electron-phonon scattering rate

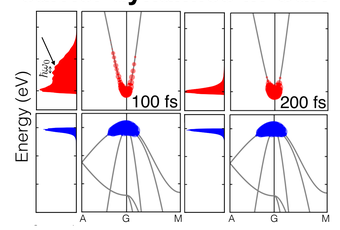
$$\Gamma_{n\mathbf{k}} = \frac{2\pi}{\hbar} \sum_{\mathbf{q}\nu m} w_{\mathbf{q}} \left| g^{\mathbf{q}\nu,mn}_{\mathbf{k}+\mathbf{q},\mathbf{k}} \right|^2 \{ [n(\omega_{\mathbf{q}\nu}) + f(\epsilon_{m\mathbf{k}+\mathbf{q}})] \delta(\epsilon_{n\mathbf{k}} - \epsilon_{m\mathbf{k}+\mathbf{q}} + \hbar\omega_{\mathbf{q}\nu}) + [n(\omega_{\mathbf{q}\nu}) + 1 - f(\epsilon_{m\mathbf{k}+\mathbf{q}})] \delta(\epsilon_{n\mathbf{k}} - \epsilon_{m\mathbf{k}+\mathbf{q}} - \hbar\omega_{\mathbf{q}\nu}) \}$$

Performance and Example Calculations

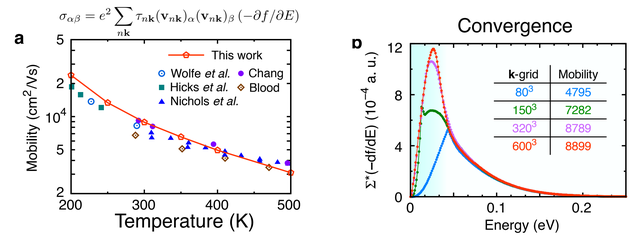
e-ph coupling coefficient



Asymmetry in the excited carrier dynamics in GaN

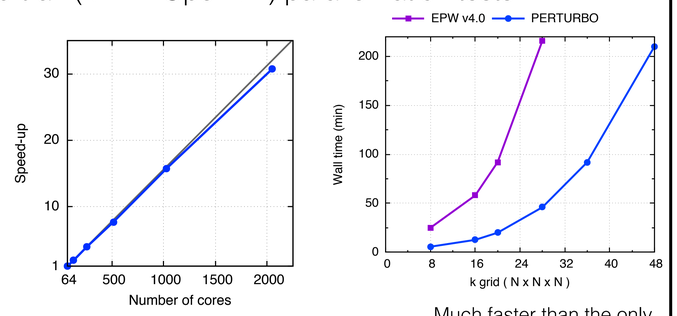


Electron mobility in GaAs



Code implementation

Fortran (MPI + OpenMP) parallelization tests



Scales up to ~10,000 cores

Much faster than the only other e-ph code (EPW)

References

- L. Agapito et al., Phys. Rev. B 93, 035104, 2016
- J.-J. Zhou and M. Bernardi, Phys. Rev. B 94, 201201(R), 2016
- M. Bernardi, Eur. J. Phys. B 89, 239, 2016
- V. Jhalani, J.-J. Zhou, and M. Bernardi (Submitted)

Acknowledgments

NSF NERSC XSEDE Extreme Science and Engineering Discovery Environment